Isomenthyl-derived 1,3-diol ligands catalyzing an asymmetric aldol reaction identified through parallel synthesis and screening

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Contents:

HPLC Data for Mukaiyama aldol products from parallel catalyst screen. Ligand generated in situ in each reaction tube is shown.

NMR (1H, 13C, HMBC) for pure reference sample of Mukaiyama aldol product prepared using achiral conditions. This sample confirmed peaks by HPLC to represent enantiomers.

NMR data for independently prepared examples of 2 isomenthene aldol constituents included in the parallel synthesis sequence, and of 2 independently prepared examples of the diols included of the ligand array.
NMR Data for racemic Mukaiyama aldol product

(±)
NMR Data for independently prepared isomenthone aldol products and diols

Data for single diastereomer:
configuration unassigned
(reaction generates 80:20)
data for single diastereomer:
configuration unassigned
(reaction generates 80:20)